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MULTI-STEP RUNGE-KUTTA METHODS

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MULTI-STEP RUNGE-KUTTA METHODS

SUMMARY

The multi-step methods presented in this report differ from the classic, single-step Runge-Kutta process by utilizing the numerical results of the previous integrations. As developed here, the multi-step process avoids the complex Taylor expansions of the functions involved and instead employs the writer's previously developed method of quadratures.

INTRODUCTION

The classic Runge-Kutta method, which is a single-step process, has a number of pleasing properties, but since it does not utilize previous numerical results of the integration, its efficiency is impaired. This defect will be somewhat remedied here by developing a multi-step method that is quite analogous to the single-step Runge-Kutta process. By utilizing the evaluations at preceding points of the function in the differential equation to be integrated, some reduction in the number of evaluations required in the single-step process is expected.

Perhaps the greatest obstacle in the development of a multi-step process is the tedious--and formidable--task of making Taylor expansions of the functions (those for both the current and preceding points) about the current point. In a recent article [1], the writer has developed a "method of quadratures" for obtaining the system of equations that determine the parameters of the (single-step) classic Runge-Kutta process; this method obviates the need for making the complex Taylor expansions. In this report we will show how the method of quadratures can be extended to the multi-step process.

THE TWO-STEP FOURTH-ORDER SOLUTION

For simplicity, we will consider only the initial value problem

$$y' = f(x,y) \quad y(x_0) = y_0$$
 (1)

though the results may be extended to systems of differential equations. We define the sequence of equations

$$k_1^{(0)} = hf(x_0, y_0)$$
 (2a)

$$k_2^{(0)} = hf \left(x_0 + \alpha_2 h, y_0 + \beta_{21} k_1^{(0)} \right)$$
 (2b)

$$k_3^{(0)} = hf\left(x_0 + \alpha_3 h, y_0 + \beta_{31}k_1^{(0)} + \beta_{32}k_2^{(0)}\right)$$
 (2c)

where x_0 and y_0 designate the current point.

Let

$$x_{-1} = x_0 - h$$

 $y_{-1} = y(x_0 - h)$ (3)

refer to the preceding point separated by the step-size h. If we replace x_0 , y_0 in equation (2) by x_{-1} and y_{-1} (and make the appropriate changes in the superscripts on the k's), we get

$$k_1^{(-1)} = hf (x_0 - h, y_{-1})$$
 (4a)

$$k_2^{(-1)} = hf \left(x_0 + (\alpha_2 - 1) h, y_{-1} + \beta_{21} k_1^{(-1)} \right)$$
 (4b)

$$k_3^{(-1)} = hf\left(x_0 + (\alpha_3 - 1)h, y_{-1} + \beta_{31}k_1^{(-1)} + \beta_{32}k_2^{(-1)}\right)$$
 (4c)

In equations (2) and (4), and subsequently, the superscripts will distinguish the current from the preceding point.

We will show that

$$y(x_0 + h) \approx y_0 + \omega_1^{(0)} k_1^{(0)} + \omega_2^{(0)} k_2^{(0)} + \omega_3^{(0)} k_3^{(0)} + \omega_1^{(-1)} k_1^{(-1)} + \omega_2^{(-1)} k_2^{(-1)} + \omega_3^{(-1)} k_3^{(-1)}$$

$$(5)$$

with appropriate values for the weights and the parameters in equations (2) and (4), will give a solution of fourth-order accuracy at $(x_0 + h)$. Since

the evaluations of the functions in equation (4) will already have been made, 1 only the three evaluations in equation (2) will be required to find the solution at the next point $(x_0 + h)$. Because these evaluations are the most time-consuming part of the computation and since the classic Runge-Kutta theory required four evaluations for this order, 2 the advantage of this multi-step method is evident.

Suppose now that equation (1) is reformulated as

$$y(x_0 + h) - y(x_0) = \int_{x_0}^{x_0 + h} f(x, y(x)) dx$$
 (6)

in which form it includes the initial conditions. Now let us replace the right member of equation (6) by the approximating quadrature sum

h
$$\left[\omega_{1}^{(0)} f(x_{0}, y_{0}) + \omega_{2}^{(0)} f(x_{1}, y_{1}) + \omega_{3}^{(0)} f(x_{2}, y_{2}) + \omega_{1}^{(-1)} f(x_{-1}, y_{-1}) + \omega_{2}^{(-1)} f(x_{-2}, y_{-2}) + \omega_{3}^{(-1)} f(x_{-3}, y_{-3})\right]$$

where for convenience we have set

$$x_1 = x_0 + \alpha_2 h$$

$$x_2 = x_0 + \alpha_3 h$$
(8)

and

$$x_{-1} = x_0 - h$$

$$x_{-2} = x_0 + (\alpha_2 - 1)h$$

$$x_{-3} = x_0 + (\alpha_3 - 1)h$$
(9)

and where y_i will be used for $y(x_i)$. We will now show how we may replace each term in equation (7) by its corresponding term in equation (5).

¹Except initially. Thus, in common with all multi-step methods, it is not self-starting.

²This assumes that the errors in the two cases are comparable--which need not be the case.

As we have shown in [1], in order for equation (7) to be a quadrature approximation of equation (6) with fourth-order accuracy in h, the following relations must hold:

$$h(\omega_{1}^{(-1)}\omega_{2}^{(-1)}\omega_{3}^{(-1)}|_{\omega_{1}}^{j}(0)\omega_{2}^{(0)}\omega_{3}^{(0)}) = \begin{pmatrix} x_{-1}^{j} \\ x_{-2}^{j} \\ -x_{0}^{-\frac{1}{3}} - x_{0}^{j} \\ x_{1}^{j} \\ x_{2}^{j} \end{pmatrix} = u_{j}, \quad j=0,1,2,3$$
(10)

where u is given by

$$u_{j} = \int_{X_{0}}^{X_{0}+h} x^{j} dx = \frac{(x_{0}+h)^{j+1} x_{0}^{j+1}}{j+1}, \quad j = 0, 1, 2, 3$$
 (11)

The reason for showing the partitions in the matrices in equation (10) is evident.

If we substitute equations (8), (9), and (11) into equation (10) and equate coefficients of like powers of h, we get the matrix equation that may replace equation (10) 3

³See reference [1] for more details about this operation.

These give some of the equations in the multi-step Runge-Kutta process.

Using the quadrature method, let us now examine the further conditions by which equation (7) may be replaced by equation (5). If we compare analogous terms in equations (5) and (7) we see that the differences are in the expressions that replace y_i in the functions $f(x_i, y_i)$; the substitutions for y_i , shown in equations (2) and (4), substantially represent the unique aspect of the Runge-Kutta process. These interchanges for the y_i in $f(x_i, y_i)$ might be permissible if the terms in equation (7) are replaced by expressions of an acceptable order, the order three in this case, not four, because of the factor h in both equations (5) and (7). To attain this precision certain conditions, which will give other Runge-Kutta equations, must be imposed.

Thus, the first term in equation (7) that will be affected by substituting replacements for y_i is $f(x_1, y_1)$, which is to be replaced by

$$f\left(x_0 + \alpha_2 h, y_0 + \beta_{21} k_1^{(0)}\right)$$
 (13)

as may be seen from equation (2b). This may be done by making a quadrature approximation for y_1 that replaces it with $(y_0 + \beta_{21}k_1^{(0)})$, as is shown in equation (13); to attain the requisite precision indicated previously, the following conditions must hold [1]:

$$(h \beta_{21}) x_0^0 = u_0(\alpha_2)$$

$$(h \beta_{21}) x_0 = u_1(\alpha_2)$$

$$(h \beta_{21}) x_0^2 = u_2(\alpha_2)$$

$$(h \beta_{21}) x_0^3 = u_3(\alpha_2)$$
(14)

where

$$u_{r}(\alpha_{i+1}) = \int_{X_{0}}^{X_{0} + \alpha_{i+1}h} x^{r} dx = \frac{(x_{0} + \alpha_{i+1}h)^{r+1} - x_{0}^{r+1}}{r+1}$$
(15)

Similarly, to replace $f(x_{-2}, y_{-2})$ in equation (7) by $f(x_{-2}, y_{-1} + \beta_{21}k_1^{(-1)})$, as shown in equation (4b), with the necessary precision, we must also satisfy the conditions

$$(h\beta_{21}) \quad (x_0 - h)^0 = \overline{u}_0(\alpha_2)$$

$$(h\beta_{21}) \quad (x_0 - h)^1 = \overline{u}_1(\alpha_2)$$

$$(h\beta_{21}) \quad (x_0 - h)^2 = \overline{u}_2(\alpha_2)$$

$$(h\beta_{21}) \quad (x_0 - h)^3 = \overline{u}_3(\alpha_3)$$

$$(16)$$

where

$$\overline{u}_{r}(\alpha_{i+1}) = \int_{x_{0}-h}^{x_{0}+(\alpha_{i+1}-1)h} x^{r} dx = \frac{\left[x_{0}+(\alpha_{i+1}-1)h\right]^{r+1}-\left(x_{0}-h\right)^{r+1}}{r+1}$$

$$r = 0,1,2,3 \tag{17}$$

As may easily be seen , equations (16) and (17) can be obtained simply by replacing x_0 by $(x_0 - h)$ in equations(14) and (15); this is to be expected if we note that equation (4b) is obtained from equation (2b) by the same transformation.

Similarly, we can replace $f(x_2, y_2)$ and $f(x_{-3}, y_{-3})$ in equation (7) by the functions shown in equations (2c) and (4c); this is accomplished by replacing y_2 and y_{-3} with appropriate quadratures.

The conditions for replacing y_2 by $(y_0 + \beta_{31}k_1^{(0)} + \beta_{32}k_2^{(0)})$, as shown in equation (2c) and with the requisite degree of precision three, are

$$(h\beta_{31}) x_0^0 + (h\beta_{32}) x_1^0 = u_0(\alpha_3)$$

$$(h\beta_{31}) x_0 + (h\beta_{32}) x_1 = u_1(\alpha_3)$$

$$(h\beta_{31}) x_0^2 + (h\beta_{32}) x_1^2 = u_2(\alpha_3)$$

$$(h\beta_{31}) x_0^3 + (h\beta_{32}) x_1^3 = u_3(\alpha_3)$$

$$(18)$$

where $u_r(\alpha_3)$ is given by equation (15).

Similarly, to replace y_{-3} in $f(x_{-3}, y_{-3})$ by $(y_{-1} + \beta_{31}k_1^{(-1)} + \beta_{32}k_2^{(-1)})$, as is indicated in equation (4c), with the required degree of precision, we must satisfy

$$(h\beta_{31}) + (h\beta_{32}) = \overline{u}_{0}(\alpha_{3})$$

$$(h\beta_{31}) (x_{0} - h) + (h\beta_{32})x_{0} = \overline{u}_{1}(\alpha_{3})$$

$$(h\beta_{31}) (x_{0} - h)^{2} + (h\beta_{32})x_{0}^{2} = \overline{u}_{2}(\alpha_{3})$$

$$(h\beta_{31}) (x_{0} - h)^{3} + (h\beta_{32})x_{0}^{3} = \overline{u}_{3}(\alpha_{3})$$

$$(19)$$

where $\bar{u}_r(\alpha_3)$ is given by equation (17). As before, we can see that equation (19) can be obtained from equation (18) by replacing x_0 with $(x_0 - h)$ -- and, of course, x_1 with x_0 -- with corresponding changes in the right members.

THE RUNGE-KUTTA MATRIX EQUATION

In [1] we have shown, for the classic single-step case, how the conditions we derived by using our quadrature method--in this present case the analogous equations (14), (16), (18), and (19)--are used to give an applicable Runge-Kutta matrix equation.

We will here reconstruct the general idea without too detailed a treatment (see also Appendix A). Using the aforementioned equations, let us form the following weighted expressions:

$$\omega_{2}^{(-1)}\overline{u}_{j}(\alpha_{2}) + \omega_{3}^{(-1)}\overline{u}_{j}(\alpha_{3}) + \omega_{2}^{(0)}u_{j}(\alpha_{2}) + \omega_{3}^{(0)}u_{j}(\alpha_{3}), j=0,1,2,3$$
 (20)

Let us first dispose of the case j=0. We must first note, by equations (15) and (17), that

$$u_0 (\alpha_{i+1}) = \overline{u}_0 (\alpha_{i+1}) = \alpha_{i+1} h$$

so that the first equations in (14), (16), (18), and (19) are identically

satisfied if

$$\alpha_2 = \beta_{21}$$

$$\alpha_3 = \beta_{31} + \beta_{32}$$

In general, the equations

$$\alpha_{i+1} = \beta_{i+1,1} + \beta_{i+2,2} + \dots + \beta_{i+1,i}, \quad i=1,2 \quad (N-1)$$
 (21)

hold as they do in the single-step case.

Let us illustrate the result of using equation (20) when j=2. Using equations (15) and (17) to replace the u_i 's, we have

$$(x_0^{2}h) \left\{ \omega_2^{(-1)} \alpha_2 + \omega_3^{(-1)} \alpha_3 + \omega_2^{(0)} \alpha_2 + \omega_3^{(0)} \alpha_3 \right\}$$

$$(2x_0h^2) \left\{ \omega_2^{(-1)} \left(-\alpha_2 + \frac{1}{2}\alpha_2^2 \right) + \omega_3^{(-1)} \left(-\alpha_3 + \frac{1}{2}\alpha_3^2 \right) + \omega_2^{(0)} \left(\frac{1}{2}\alpha_2^2 \right) \right.$$

$$\left. + \omega_3^{(0)} \left(\frac{1}{2}\alpha_3^2 \right) \right\} + (h^3) \left\{ \omega_2^{(-1)} \left(\frac{1}{3}\alpha_2^3 - \alpha_2^2 + \alpha_2 \right) \right.$$

$$\left. + \omega_3^{(-1)} \left(\frac{1}{3}\alpha_3^3 - \alpha_3^2 + \alpha_3 \right) + \omega_2^{(0)} \left(\frac{1}{3}\alpha_2^3 \right) + \omega_3^{(0)} \left(\frac{1}{3}\alpha_3^3 \right) \right\}$$

$$(22)$$

The corresponding expression for (20) is as follows, ⁴ if we replace $u_2(\alpha_2)$, $u_2(\alpha_3)$ and $\bar{u}_2(\alpha_2)$, $\bar{u}_2(\alpha_3)$ by the left members of the equations (14), (16), (18), and (19):

$$\begin{aligned} &(\mathbf{x_0}^{2}\mathbf{h}) \quad \left\{ \omega_{2}^{-1}\alpha_{2} + \omega_{3}^{-1}\alpha_{3} + \omega_{2}^{0}\alpha_{2} + \omega_{3}^{0}\alpha_{3} \right\} \\ &+ (2\mathbf{x_0}\mathbf{h}^{2}) \left\{ \omega_{2}^{(-1)} \left(-\alpha_{2} \right) + \omega_{3}^{(-1)} (\beta_{32}\alpha_{2} - \alpha_{3}) + \omega_{2}^{(0)} \right\} \\ &+ (\mathbf{h}^{3}) \left\{ \omega_{2}^{(-1)}\alpha_{2} + \omega_{3}^{(-1)} (\beta_{32}\alpha_{2}^{2} - 2\beta_{32}\alpha_{2} + \alpha_{3}) + \omega_{2}^{(0)} \right\} \\ &+ \omega_{3}^{(0)} \left(\beta_{32}\alpha_{2}^{2} \right) \right\} \end{aligned}$$

$$(23)$$

If now we equate powers of h in equations (22) and (23), we obtain the two Runge-Kutta equations:

$$\omega_2^{(-1)}\alpha_2^2 + \omega_3^{(-1)} (\alpha_3^2 - 2\beta_{32}\alpha_2) + \omega_2^{(0)}\alpha_2^2 + \omega_3^{(0)} (\alpha_3^2 - 2\beta_{32}\alpha_2) = 0$$
(24)

⁴We omit the h term since it contributes nothing new.

$$\omega_{2}^{(-1)} \left(-\alpha_{2}^{3} + 3\alpha_{2}^{2}\right) + \omega_{3}^{(-1)} \left(-\alpha_{3}^{3} + 3\alpha_{3}^{2} + 3\beta_{32}\alpha_{2}^{2} - 6\beta_{32}\alpha_{2}\right) - \omega_{2}^{(0)}\alpha_{2}^{3} + \omega_{3}^{(0)} \left(3\beta_{32}\alpha_{2}^{2} - \alpha_{3}^{3}\right) = 0$$
(25)

No new results will be derived if we treat equation (20) similarly when j = 1, 3.

Without repeating in detail what has been developed in [1] for the single-step classic Runge-Kutta process, we will note that we can replace $\omega_{\bf i}^{(0)}$ in equation (20) by $\omega_{\bf i}^{(0)}$ $\alpha_{\bf i}$ and, similarly, $\omega_{\bf i}^{(-1)}$ by $\omega_{\bf i}^{(-1)}$ ($\alpha_{\bf i}$ - 1). A repetition of the previous analysis will yield another Runge-Kutta equation.

We will see that, as in the single-step process, if we can find other sets of what we have called generalized Runge-Kutta weight coefficients to use in equation (20) we should eventually be able to produce all of the relevant Runge-Kutta equations. We will next show how we can get all of these coefficients from the single-step process and avoid the basic, but tedious, work in the illustration above.

We will anticipate the results we would obtain in the form of a matrix equation: 5

$$\begin{pmatrix}
\omega_{2}^{(-1)} & \omega_{3}^{(-1)} & \omega_{2}^{(0)} & \omega_{3}^{(0)} \\
\omega_{2}^{(-1)} & (\alpha_{2}-1) & \omega_{3}^{(-1)} & (\alpha_{3}-1) & \omega_{2}^{(0)} & \alpha_{2} & \omega_{3}^{(0)} \\
\omega_{3}^{(-1)} & \beta_{32} & 0 & \omega_{3}^{(0)} & \beta_{32} & 0
\end{pmatrix}
\begin{pmatrix}
-\frac{1}{2} & \alpha_{2}^{2} & -\alpha_{2}^{2} & (\frac{1}{3} & \alpha_{2}-1) \\
\beta_{32} & \alpha_{2}-\frac{1}{2} & \alpha_{3}^{2} & (\beta_{32} & \alpha_{2}^{2}-\frac{1}{3} & \alpha_{3}^{3} & -2\beta_{32} & \alpha_{2} + \alpha_{3}^{2}) \\
-\frac{1}{2} & \alpha_{2}^{2} & -\frac{1}{3} & \alpha_{3}^{2} \\
\beta_{32} & \alpha_{2}-\frac{1}{2} & \alpha_{3}^{2} & (\beta_{32} & \alpha_{2}^{2}-\frac{1}{3} & \alpha_{3}^{3})
\end{pmatrix}$$

$$(26)$$

where 0, the right member of equation (26), is the appropriate null matrix.

THE TWO-STEP FIFTH-ORDER RUNGE-KUTTA EQUATIONS

The process for obtaining the generalized Runge-Kutta weight matrix, even for the relatively simple two-step fourth-order case, becomes somewhat

⁵As we will see later only four of these equations are relevant. The solution for the two-step fourth order is given in Appendix B.

involved when rigorously justified. We will now examine a procedure that is an extension of the one-step process, and that can easily be extended to any order, as is seen in [1]. Let us demonstrate this by developing the two-step fifth-order Runge-Kutta matrix equation. With a slight modification of the results derived in [1], we will first write out the one-step Runge-Kutta matrix equation for the fifth order with five evaluations. ⁶

Let us define the matrices

$$\Omega^{(0)} = \begin{pmatrix} \omega_{2} & \cdot & \cdot & \omega_{5} \\ \omega_{2}\alpha_{2} & \cdot & \cdot & \omega_{5}\alpha_{2} \\ \omega_{2}\alpha_{2}^{2} & \cdot & \cdot & \omega_{5}\alpha^{2} \\ \gamma_{2}^{(0)} & \cdot & \cdot & \gamma_{5}^{(0)} \\ \gamma_{2}^{(0)}\alpha_{2} & \cdot & \cdot & \gamma_{5}^{(0)} \\ \gamma_{2}^{(1)} & \cdot & \cdot & \gamma_{5}^{(1)} \\ \omega_{2}c_{2}^{(1)} & \cdot & \cdot & \omega_{5}c_{5}^{(1)} \\ \gamma_{2}^{(0)}(\gamma_{1}^{0}) & \cdot & \cdot & \gamma_{5}^{(0)}(\gamma_{1}^{(0)}) \end{pmatrix}$$
 and
$$C = \begin{pmatrix} c_{1}^{(1)} & c_{2}^{(2)} & c_{2}^{(3)} \\ c_{3}^{(1)} & c_{3}^{(2)} & c_{3}^{(3)} \\ c_{4}^{(1)} & c_{4}^{(2)} & c_{4}^{(3)} \\ c_{5}^{(1)} & c_{5}^{(2)} & c_{5}^{(3)} \end{pmatrix}$$
 (28)

⁶The exact number of evaluations is unimportant for our demonstration.

where

where
$$(\omega_{3}\alpha_{3}^{n} \quad \omega_{4}\alpha_{4}^{n} \quad \omega_{5}\alpha_{5}^{n}) \quad \begin{pmatrix} \beta_{32} & 0 & 0 & 0 \\ \beta_{42} & \beta_{43} & 0 & 0 \\ \beta_{52} & \beta_{53} & \beta_{54} & 0 \end{pmatrix} = \begin{pmatrix} \gamma_{2}^{(n)}\gamma_{3}^{(n)}\gamma_{4}^{(n)}\gamma_{5}^{(n)} \end{pmatrix},$$

$$n = 0, 1 \qquad (29)$$

$$c_{2}^{(j)} = 0$$

$$c_{3}^{(j)} = \beta_{32}\alpha_{2}^{j}$$

$$c_{4}^{(j)} = \beta_{42}\alpha_{2}^{j} + \beta_{43}\alpha_{3}^{j}$$

$$c_{5}^{(j)} = \beta_{52}\alpha_{2}^{j} + \beta_{53}\alpha_{3}^{j} + \beta_{54}\alpha_{4}^{j}, \quad j = 1, 2, 3$$
(30)

and where⁷

$$\gamma_{2}^{(0)} (\gamma_{1}) = (\omega_{4}\beta_{43} + \omega_{5}\beta_{53}) \beta_{32} + (\omega_{5}\beta_{54}) \beta_{42} + \gamma_{5}^{(0)}\beta_{52}$$

$$\gamma_{3}^{(0)} (\gamma_{1}) = \gamma_{4}^{(0)}\beta_{43} + \gamma_{5}^{(0)}\beta_{53}$$

$$\gamma_{4}^{(0)} (\gamma_{1}) = \gamma_{5}^{(0)}\beta_{54} = 0$$

$$\gamma_{5}^{(0)} (\gamma_{1}) = 0$$

The single-step fifth-order Runge-Kutta matrix equation with five evaluations⁸ is given by

$$\Omega^{(0)}\chi^{(0)} = 0 \tag{31}$$

defined by equation (29), by replacing ω_{i} in the latter terms with the corresponding $\gamma_i^{(0)}$.

⁸It has been shown [2, 3] that the fifth order requires at least six evaluations for a solution. Since we are using a two-step process, we would like to reduce the number of evaluations by one.

⁷The values for $\gamma_i^{(0)}(\gamma_i)$, (j = 2,3,4,5) may be derived from $\gamma_i^{(0)}(\omega_i)$,

where 0 is the appropriate null matrix and where

$$\chi^{(0)} = C - \begin{pmatrix} \frac{1}{2}\alpha_2^2 & \frac{1}{3}\alpha_2^3 & \frac{1}{4}\alpha_2^4 \\ \frac{1}{2}\alpha_3^2 & \frac{1}{3}\alpha_3^3 & \frac{1}{4}\alpha_3^4 \\ \frac{1}{2}\alpha_4^2 & \frac{1}{3}\alpha_4^3 & \frac{1}{4}\alpha_4^4 \\ \frac{1}{2}\alpha_5^2 & \frac{1}{3}\alpha_5^3 & \frac{1}{4}\alpha_5^4 \end{pmatrix}$$
(32)

and C is given by equation (28). Combining the matrices in equation (32), we get

$$\chi^{(0)} = \begin{pmatrix} \begin{bmatrix} & -\frac{1}{2}\alpha_{2}^{2} \end{bmatrix} \begin{bmatrix} & -\frac{1}{3}\alpha_{2}^{3} \end{bmatrix} \begin{bmatrix} & -\frac{1}{4}\alpha_{2}^{4} \end{bmatrix} \\ [\beta_{32}\alpha_{2} & -\frac{1}{2}\alpha_{3}^{2} \end{bmatrix} \begin{bmatrix} \beta_{32}\alpha_{2}^{2} & -\frac{1}{3}\alpha_{3}^{3} \end{bmatrix} [\beta_{32}\alpha_{2}^{3} & -\frac{1}{4}\alpha_{4}^{4} \end{bmatrix} \\ [(\beta_{42}\dot{\alpha}_{2} + \beta_{43}\alpha_{3} & -\frac{1}{2}\alpha_{4}^{2} \end{bmatrix} \begin{bmatrix} (\beta_{42}\alpha_{2}^{2} + \beta_{43}\alpha_{3}^{2}) & -\frac{1}{3}\alpha_{4}^{3} \end{bmatrix} [\beta_{42}\alpha_{2}^{3} + \beta_{43}\alpha_{3}^{3} & -\frac{1}{4}\alpha_{4}^{4} \end{bmatrix} \\ [(\beta_{52}\alpha_{2} + \beta_{53}\alpha_{3} + \beta_{54}\alpha_{4}) - \frac{1}{2}\alpha_{5}^{5} \end{bmatrix} \begin{bmatrix} (\beta_{52}\alpha_{2}^{2} + \beta_{53}\alpha_{3}^{2} + \beta_{53}\alpha_{4}^{2}) - \frac{1}{3}\alpha_{5}^{3} \end{bmatrix} [(\beta_{52}\alpha_{2}^{3} + \beta_{53}\alpha_{3}^{3} + \beta_{54}\alpha_{4}^{3}) - \frac{1}{4}\alpha_{5}^{4} \end{bmatrix} \end{pmatrix}$$

The two-step fifth-order Runge-Kutta process with five evaluations will take the linear form

$$y(x_0 + h) \approx y_0 + \sum_{i=1}^{5} \omega_i^{(-1)} k_i^{(-1)} + \sum_{i=1}^{5} \omega_i^{(0)} k_i^{(0)}$$
 (34)

where

$$k_{i}^{(0)} = hf\left(x_{0} + \alpha_{i} h, y_{0} + \sum_{j=1}^{i-1} \beta_{ij} k_{j}^{(0)}\right)$$
 (35)

$$k_i^{(-1)} = hf \left[x_0 + (x_i^{-1})h, y_{-1} + \sum_{j=1}^{i-1} \beta_{ij} k_j^{(-1)} \right]$$
 (36)

and where the superscripts (0) and (-1) refer to the current and preceding points, respectively.

To accommodate the antecedent point, certain modifications will have to be made in the two matrices in equation (31). In the case of the matrix $\Omega^{(0)}$, as we may see from equation (26), this is quite simple because, aside from the appropriate superscript on ω_i , we must replace α_i by $(\alpha_i$ -1). With these changes we will call the resulting matrix $\Omega^{(-1)}$.

The accompanying change in the matrix in equation (33) is not as simple, and only the result will be given for the order of interest here. 9 Thus, if we write for the matrix in equation (33)

$$\chi^{(0)} = \begin{pmatrix} e_{11} & e_{21} & e_{31} \\ e_{12} & e_{22} & e_{32} \\ e_{13} & e_{23} & e_{33} \\ e_{14} & e_{24} & e_{34} \end{pmatrix}$$

$$(37)$$

we should replace this by

$$\chi^{(-1)} = \begin{pmatrix} e_{11} & (e_{21} - 2e_{11}) & (e_{31} + 3e_{11} - 3e_{21}) \\ e_{12} & (e_{22} - 2e_{12}) & (e_{32} + 3e_{12} - 3e_{22}) \\ e_{13} & (e_{23} - 2e_{13}) & (e_{33} + 3e_{13} - 3e_{23}) \\ e_{14} & (e_{24} - 2e_{14}) & (e_{34} + 3e_{14} - 3e_{24}) \end{pmatrix}$$

$$(38)$$

or, substituting the values for the elements from equation (33) and using the superscript (-1) to distinguish it from the matrix for the current point, we have

⁹This is developed in detail in Appendix A.

$$\mathbf{x}^{(-1)} = \begin{pmatrix} \begin{bmatrix} -\frac{1}{2}\alpha_{2}^{2} \end{bmatrix} & \begin{bmatrix} -\frac{1}{3}\alpha_{2}^{3} + \alpha_{2}^{2} \end{bmatrix} & \begin{pmatrix} -\frac{1}{4}\alpha_{2}^{4} - \frac{3}{2}\alpha_{2}^{2} + \alpha_{2}^{3} \end{pmatrix} \\ \begin{bmatrix} \beta_{32}\alpha_{2} & -\frac{1}{2}\alpha_{3}^{2} \end{bmatrix} & \begin{pmatrix} \beta_{32}\alpha_{2}^{2} - \frac{1}{2}\alpha_{3}^{3} - \beta_{32}\alpha_{2} + \alpha_{3}^{2} \end{pmatrix} & \begin{bmatrix} \left(\beta_{32}\alpha_{2}^{3} - \frac{1}{4}\alpha_{3}^{4} + 3\beta_{32}\alpha_{2} - \frac{3}{2}\alpha_{3}^{2} - 3\beta_{32}\alpha_{2}^{2} + \alpha_{3}^{2} \end{pmatrix} \end{bmatrix} \\ \begin{bmatrix} (\beta_{43}\alpha_{2} + \beta_{43}\alpha_{3}) & -\frac{1}{2}\alpha_{4}^{2} \end{bmatrix} & \begin{bmatrix} \left(\beta_{42}\alpha_{2}^{2} + \beta_{43}\alpha_{3}^{2} - \frac{1}{3}\alpha_{4}^{3} \right) \\ -2\left(\beta_{42}\alpha_{2} + \beta_{43}\alpha_{3} - \frac{1}{2}\alpha_{4}^{2} \right) \end{bmatrix} & -\frac{3}{2}\alpha_{3}^{2} - 3\beta_{32}\alpha_{2}^{2} + \alpha_{3}^{2} \end{pmatrix} \end{bmatrix} \\ \begin{bmatrix} (\beta_{52}\alpha_{2} + \beta_{53}\alpha_{3} + \beta_{54}\alpha_{4}) & -\frac{1}{2}\alpha_{5}^{2} \end{bmatrix} & -\frac{3}{2}\alpha_{3}^{2} - 3\beta_{32}\alpha_{2}^{2} + \alpha_{3}^{2} \end{pmatrix} \end{bmatrix}$$

$$(39)$$

whose elements are partially shown in equation (39).

We can now combine our results to give us the matrix equation for the two-step fifth-order process. This can be written

$$\left(\Omega^{(-1)} \middle| \Omega^{(0)}\right) \left(\begin{matrix} --\frac{\chi}{\sqrt{(0)}} \\ -\frac{\chi}{\sqrt{(0)}} \end{matrix}\right) = 0 \tag{40}$$

where the partitioned matrices shown are as previously defined and 0 is an appropriate null matrix.

As an illustration, let us return to the two-step fourth-order equations with three evaluations at each point, then the matrices in equation (40) become

$$\begin{pmatrix} \omega_{2}^{(-1)} & \omega_{3}^{(-1)} & | & \omega_{2}^{(0)} & \omega_{3}^{(0)} \\ \omega_{2}^{(-1)}(\alpha_{2}-1) & \omega_{3}^{(-1)}(\alpha_{3}-1) & | & \omega_{2}^{(0)}\alpha_{2} & \omega_{3}^{(0)}\alpha_{3} \\ \omega_{2}^{(-1)}(\alpha_{2}-1) & \omega_{3}^{(-1)}(\alpha_{3}-1) & | & \omega_{2}^{(0)}\alpha_{2} & \omega_{3}^{(0)}\alpha_{3} \\ \omega_{2}^{(-1)}(\alpha_{2}-1) & \omega_{3}^{(-1)}(\alpha_{3}-1) & | & \omega_{2}^{(0)}\alpha_{2} & \omega_{3}^{(0)}\alpha_{3} \\ \omega_{3}^{(-1)}\beta_{32} & 0 & | & \omega_{3}^{(0)}\beta_{32} & 0 \\ \omega_{3}^{(-1)}\beta_{32} & 0 & | & \omega_{3}^{(0)}\beta_{32} & 0 \\ \omega_{3}^{(-1)}\beta_{32}(\alpha_{2}-1) & 0 & | & \omega_{3}^{(0)}\beta_{32}\alpha_{2} & 0 \\ \omega_{3}^{(-1)}\beta_{32}(\alpha_{3}-1) & 0 & | & \omega_{3}^{(0)}\beta_{32}\alpha_{3} & 0 \\ 0 & \omega_{3}^{(-1)}\beta_{32}(\alpha_{2}-1) & | & 0 & \omega_{3}^{(0)}\beta_{32}\alpha_{3} & 0 \\ \end{pmatrix} \begin{pmatrix} -\frac{1}{2}\alpha_{2}^{2} & -\alpha_{2}^{2}\left(\frac{1}{3}\alpha_{2}-1\right) & -\alpha_{2}^{2}\left(\frac{1}{4}\alpha_{3}^{2}-\alpha_{2}+\frac{3}{2}\right) \\ \beta_{32}\alpha_{2}^{2}-\frac{1}{3}\alpha_{3}^{2} & | & (\beta_{32}\alpha_{2}^{2}-\frac{1}{3}\alpha_{3}^{2}) & [\beta_{32}\alpha_{2}^{2}-\frac{1}{4}\alpha_{3}^{2}] & -\beta_{32}\alpha_{2}^{2}+\alpha_{3}^{2}] \end{pmatrix} = 0$$

which give both the Runge-Kutta equations for the fourth-order method¹⁰ and the fifth-order terms from which we may find the truncation error. ¹¹ If the latter terms are ignored, equation (41) will adequately represent the required equations.

George C. Marshall Space Flight Center
National Aeronautics and Space Administration
Huntsville, Alabama, September 1, 1967
039-00-24-0000

¹⁰These are the equations in which the sum of the exponents in the product of the α 's and β 's in any term is always less than the order of the process.

¹¹These equations, aside from some misprints, may be found in [4].

APPENDIX A

DERIVATION OF THE TWO-STEP FOURTH-ORDER EQUATIONS

The conditions we have derived using the quadrature methods for the two-step fourth-order process are given by equations (14), (16), (18), and (19). We will now display these equations in an expanded form in Table I and show how we can obtain from these the Runge-Kutta equations.

In the first two groups of Table I are given the equations (14) and (18) for $i=0,\ 1,\ 2,\ 3$, with the u_i (α_2) and u_i (α_3) terms in the right members expanded by using equation (15). In the last two groups in Table I are the expanded equations (16) and (19), where these are obtained from the first two groups by replacing x_0 by x_0-h .

In Table II are shown the results of combining similar terms of the left and right members of the equations in Table I. For convenience, in forming equation (20) we have associated each group in these tables with a weight coefficient $\omega_{\bf i}^{(0)}$ or $\omega_{\bf i}^{(-1)}$; and in Table I we have retained the origin of each equation by the appropriate label ${\bf u}_{\bf i}$ (α_2) or ${\bf u}_{\bf i}$ (α_3).

With the aid of Table II it is quite easy to form the expressions for equation (20) and to derive the matrix equation (26).

It will be observed that by extending Table I the Runge-Kutta equations for any higher order multi-step process may be obtained in a similar manner.

TABLE I. THE CONDITIONS FOR THE TWO-STEP FOURTH-ORDER PROCESS GIVEN BY EQUATIONS (14), (16), (18), AND (19).

$$h\beta_{21} = h\alpha_{2}$$

$$(x_{0}h)\beta_{21} = (x_{0}h)\alpha_{2} + \frac{1}{2}h^{2}\alpha_{2}^{2}$$

$$(x_{0}^{2}h)\beta_{21} = (x_{0}^{2}h)\alpha_{2} + (x_{0}h^{2})\alpha_{2}^{2} + \frac{1}{3}h^{3}\alpha_{2}^{3}$$

$$(x_{0}^{3}h)\beta_{21} = (x_{0}^{3}h)\alpha_{2} + (\frac{3}{2}x_{0}^{2}h^{2})\alpha_{2}^{2} + (x_{0}h^{3})\alpha_{2}^{3} + \frac{1}{4}h^{4}\alpha_{2}^{4}$$

$$= u_{3}(\alpha_{2})$$

$$\alpha_{2}h = \alpha_{2}h$$

$$\alpha_{3}h = \alpha_{2}h$$

$$\alpha_{4}h = \alpha_{2}h$$

$$\alpha_{4}h = \alpha_{4}h$$

$$\alpha_{4}h = \alpha_{4}h$$

$$\alpha_{5}h = \alpha_{5}h$$

$$\alpha_{5}h = \alpha$$

$$\alpha_{3}h = \alpha_{3}h$$

$$(\alpha_{3}h) (x_{0} - h) + h^{2}(\beta_{32}\alpha_{2}) = (h\alpha_{3}) (x_{0} - h) + \frac{1}{2}h^{2}\alpha_{3}^{2}$$

$$(\alpha_{3}h) (x_{0} - h)^{2} + 2(x_{0} - h)h^{2}(\beta_{32}\alpha_{2}) + h^{3}(\beta_{32}\alpha_{2}^{2}) = (h\alpha_{3}) (x_{0} - h)^{2} + h^{2}\alpha_{3}^{2} (x_{0} - h) + \frac{1}{3}h^{3}\alpha_{3}^{3}$$

$$= \bar{u}_{1}(\alpha_{3})$$

$$(\alpha_{3}h) (x_{0} - h)^{3} + 3(x_{0} - h)^{2}h^{2}(\beta_{32}\alpha_{2}) + 3(x_{0} - h)h^{3}(\beta_{32}\alpha_{2}^{2}) + h^{4}(\beta_{32}\alpha_{2}^{3}) = (h\alpha_{3}) (x_{0} - h)^{3}$$

$$= \bar{u}_{3}(\alpha_{3})$$

$$= \bar{u}_{3}(\alpha_{3})$$

TABLE II. THE RESULTS OF COMBINING SIMILAR TERMS OF THE LEFT AND RIGHT MEMBERS OF THE EQUATIONS IN TABLE I.

$$\omega_{2}^{(0)} \qquad \begin{array}{l} h^{2}(\frac{1}{2}\alpha_{2}^{2}) \\ x_{0}h^{2}(-\alpha_{2}^{2}) + h^{3}(-\frac{1}{3}\alpha_{2}^{3}) \\ 3x_{0}^{2}h^{2}(\frac{1}{2}\alpha_{2}^{2}) + 3x_{0}h^{3}(-\frac{1}{3}\alpha_{2}^{3}) + h^{4}(\frac{1}{4}\alpha_{2}^{4}) \end{array}$$

$$\omega_{2}^{(-1)} \qquad \begin{array}{l} h^{2}(-\frac{1}{2}\alpha_{2}^{2}) \\ x_{0}h^{2}(-\frac{1}{2}\alpha_{2}^{2}) + h^{3}(-\frac{1}{3}\alpha_{2}^{3} + \alpha_{2}^{2}) \\ 3x_{0}h^{2}(-\frac{1}{2}\alpha_{2}^{2}) + 3x_{0}h^{3}(-\frac{1}{3}\alpha_{2}^{3} + \alpha_{2}^{2}) + h^{4}(-\frac{1}{4}\alpha_{2}^{4} - \frac{3}{2}\alpha_{2}^{2} + \alpha_{2}^{3}) \end{array}$$

$$\omega_{3}^{(-1)} = \begin{array}{c} h^{2}(\beta_{32}\alpha_{2} - \frac{1}{2}\alpha_{3}^{2}) \\ 2x_{0}h^{2}(\beta_{32}\alpha_{2} - \frac{1}{2}\alpha_{3}^{2}) + h^{3}(\beta_{32}\alpha_{2}^{2} - \frac{1}{3}\alpha_{3}^{3} - 2\beta_{32}\alpha_{2} + \alpha_{3}^{2}) \\ 3x_{0}^{2}h^{2}(\beta_{32}\alpha_{2} - \frac{1}{2}\alpha_{3}^{2}) + 3x_{0}h^{3}(\beta_{32}\alpha_{2}^{2} - \frac{1}{3}\alpha_{3}^{3} - 2\beta_{32}\alpha_{2} + \alpha_{3}^{2}) + h^{4}(\beta_{32}\alpha_{2}^{3} - \frac{1}{4}\alpha_{3}^{4} + 3\beta_{32}\alpha_{2} - \frac{3}{2}\alpha_{3}^{2} - \beta_{32}\alpha_{2}^{2} + \alpha_{3}^{3}) \end{array}$$

APPENDIX B

SOLUTION OF THE TWO-STEP FOURTH-ORDER EQUATIONS

The solution of the Runge-Kutta equations for the two-step fourth-order process will be indicated here, since the procedure can generally be followed in the solution of other multi-step equations.

We must satisfy the four equations in (12) and, in addition, the four applicable 12 equations in (26), which are as follows:

$$e_{11}\left(\omega_{2}^{(-1)} + \omega_{2}^{(0)}\right) + e_{12}\left(\omega_{3}^{(-1)} + \omega_{3}^{(0)}\right) = 0$$
 (1-B)

$$e_{11} \left[\omega_2^{(-1)} \left(\alpha_2 - 1 \right) + \omega_2^{(0)} \alpha_2 \right] + e_{12} \left[\omega_3^{(-1)} \left(\alpha_{3-1} \right) + \omega_3^{(0)} \alpha_3 \right] = 0$$
 (2-B)

$$\omega_2^{(-1)} (e_{21} - 2e_{11}) + \omega_3^{(-1)} (e_{22} - 2e_{12}) + \omega_2^{(0)} e_{21} + \omega_3^{(0)} e_{22} = 0$$
 (3-B)

$$e_{11} \beta_{32} \left(\omega_3^{(-1)} + \omega_3^{(0)}\right) = 0$$
 (4-B)

where e_{ij} is defined by equations (33) and (37).

From equations (4-B) and (1-B) we easily obtain

$$\omega_2^{(-1)} + \omega_2^{(0)} = 0$$

$$\omega_3^{(-1)} + \omega_3^{(0)} = 0$$
(5-B)

and if we combine these with the first equation in (12), we get also

$$\omega_1^{(-1)} + \omega_1^{(0)} = 1$$
 (6-B)

¹²These are the equations that contain only terms in which the sums of the exponents in the products of the α 's and β 's do not exceed three.

Using equation (5-B), both equations (2-B) and (3-B) can be reduced to

$$\omega_2^{\ 0} \ e_{11} + \ \omega_3^{\ 0} \ e_{12} = 0$$

or

$$\omega_3^{(0)} \left(2\beta_{32}\alpha_2\right) = \omega_2^{(0)}\alpha_2^2 + \omega_3^{(0)}\alpha_3^2 \tag{7-B}$$

Equations (5-B) and (6-B) can now be used to simplify the remaining three equations in (12), which become

$$-\omega_{1}^{(-1)} + \omega_{2}^{(0)} + \omega_{3}^{(0)} = \frac{1}{2}$$

$$\omega_{2}^{(0)} \alpha_{2} + \omega_{3}^{(0)} \alpha_{3} = \frac{5}{12}$$

$$\omega_{2}^{(0)} \alpha_{2}^{2} + \omega_{3}^{(0)} \alpha_{3}^{2} = \frac{1}{3}$$
(8-B)

This linear system in the weights can readily be solved:

$$-\omega_1^{(-1)} = \frac{6\alpha_2\alpha_3 - 5(\alpha_2 + \alpha_3) + 4}{12\alpha_2\alpha_3}$$

$$\omega_2^{(0)} = \underbrace{\frac{5\alpha_3 - 4}{12\alpha_2(\alpha_3 - \alpha_2)}} = -\omega_2^{(-1)}$$

$$\omega_3^{(0)} = \frac{4 - 5\alpha_2}{12\alpha_3(\alpha_3 - \alpha_2)} = -\omega_3^{(-1)}$$
 (9-B)

Using the last equation in (8-B), equation (7-B) reduces to

$$\beta_{32} = \frac{1}{6\omega_3^{(0)}\alpha_2}$$

so that equations (2-B) and (3-B) are also satisfied, provided

$$\beta_{32} = \frac{2\alpha_3 (\alpha_3 - \alpha_2)}{\alpha_2 (4 - 5\alpha_2)}$$
 (10-B)

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